

Snapping elastic curves as a one-dimensional analogue of two-component lipid bilayers

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Abstract. In order to study a one-dimensional analogue of the spontaneous curvature model for two-component lipid bilayer membranes we consider planar curves that are made of a material with two phases. Each phase induces a preferred curvature to the curve, and these curvatures as well as phase boundaries may lead to the development of kinks. We introduce a family of energies for smooth curves and phase fields, and we show that these energies Γ -converge to an energy for curves with a finite number of kinks. The theoretical result is illustrated by some numerical examples.

Keywords: Γ -convergence, elastic curves, phase field model, two-component membrane.

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1 Introduction and Result

Integral functionals depending on curvature are of geometric interest and arise in a variety of applications such as image processing and models for elastic lines or thin shells[18, 17, 3, 12]; in particular, they appear in the study of biological membranes.[5, 9, 16] In the spontaneous-curvature model for bilayer vesicles with two lipid components equilibrium shapes are described as surfaces minimising the energy

$$\sum_{i=1,2} \int_{\Sigma_i} a_i (H - C_i)^2 + b_i K dS + \sigma |\partial \Sigma_1| \quad (1.1)$$

among all closed surfaces $\Sigma = \Sigma_1 \cup \Sigma_2$ with fixed areas $|\Sigma_i|$ and fixed enclosed volume.[2, 11] Here H and K are the mean and Gauss curvature of the membrane surface Σ , a_i and b_i are parameters related to bending resistance of the membrane, and σ is the line tension at the component boundary $|\partial \Sigma_i|$; the spontaneous curvatures C_i are supposed to reflect an asymmetry in the membrane.

Jülicher and Lipowsky[11] study the Euler-Lagrange equations of (1.1) for axially symmetric membranes with exactly one interface represented by a point on a rotated curve. They briefly discuss the possibility of different smoothness conditions for the curve at the interface, their analysis, however, is done for smooth membranes only. Du, Wang[6] and Lowengrub, Rätz, Voigt[13] perform numerical simulations using a phase field for both the membrane and the lipid components; convergence to the sharp interface model is obtained by asymptotic analysis or under strong smoothness assumption on the limit surface.

In this paper we are interested in a one-dimensional analogue of the spontaneous-curvature model for two component vesicles. We consider curves made of a material with two phases, each of which induces a preferred bending to the curve; in contrast to the above studies for membranes we do not enforce smoothness of the curves a priori. We analyse an approximation by more regular curves, which, in particular, can be treated numerically in an easier way than the model with kinks.

More precisely, we consider closed plane curves q of fixed length L that are twice weakly differentiable and regular except for a finite number of points. These curves can be parametrised with unit speed over the circle \mathbb{S}^1 , when it is given a scaled standard metric to have length L .

We require that the squared mean curvature $\kappa_q^2 = |q''|^2$ of q is integrable, so we let

$$\mathcal{C} := \{q \in C(\mathbb{S}^1; \mathbb{R}^2) : \text{there exists a set } S_q \text{ of finitely many points s. t.} \\ q \in H^2(\mathbb{S}^1 \setminus S_q; \mathbb{R}^2), |q'| = 1 \text{ in } \mathbb{S}^1 \setminus S_q\}$$

be the set of parametrised curves which may have a finite number of kinks. Indeed, because H^2 embeds continuously in C^1 , S_q is the set of discontinuities of the tangent vector q' or, as $|q'|$ is constant, of the tangent angle. Note also that $\mathcal{C} \subset H^1(\mathbb{S}^1; \mathbb{R}^2)$.

The material phases of $q \in \mathcal{C}$ are determined by a function $v : \mathbb{S}^1 \rightarrow \{\pm 1\}$ having at most a finite number of jumps and satisfying the volume constraint

$$\int_{\mathbb{S}^1} v dt = mL \quad (1.2)$$

for fixed $m \in (-1, 1)$. We denote the set of such functions by \mathcal{P} and the jump set of $v \in \mathcal{P}$ by S_v ; note that $\mathcal{P} \subset BV(\mathbb{S}^1; \{\pm 1\})$.

On basis of the membrane model we consider for $(q, v) \in \mathcal{C} \times \mathcal{P}$ the energy

$$\mathcal{E}(q, v) := \int_{\mathbb{S}^1 \setminus (S_q \cup S_v)} (\kappa_q - C(v))^2 dt + \sum_{s \in S_q \cup S_v} (\sigma + \hat{\sigma} |[q'](s)|). \quad (1.3)$$

Compared to (1.1) we have dropped the Gauss curvature term, as curves have no intrinsic curvature. Furthermore, for notational simplicity we have set all bending rigidities to one and let only the spontaneous curvatures $C(\pm 1)$ be phase-dependent. Different rigidities can be treated similar to the spontaneous curvature below.

In (1.3) interfaces without kinks are penalised by the constant energy σ , while kinks carry an additional “bending energy” $\hat{\sigma} |[q'](s)|$ where $\hat{\sigma}$ is a constant and $|[q'](s)|$ denotes the modulus of the angle enclosed by the two one-sided tangent vectors at s modulo 2π . Note, that kinks may not only occur at interfaces, but also within a phase. Such kinks can be seen as resembling budding transitions or non-smooth limit shapes of even single-component membranes; we shall call them *ghost interfaces*.

As an approximation to this model we consider curves from the set

$$\mathcal{C}_\varepsilon := \{q \in H^2(\mathbb{S}^1; \mathbb{R}^2) : |q'| = 1 \text{ in } \mathbb{S}^1\}.$$

We replace sharp material phases by phase fields $v \in H^1(\mathbb{S}^1)$ with the constraint (1.2), denoting this set of functions by \mathcal{P}_ε . For $\varepsilon > 0$ and $(q, v) \in \mathcal{C}_\varepsilon \times \mathcal{P}_\varepsilon$ we consider the energy

$$\mathcal{E}_\varepsilon(q, v) := \int_{\mathbb{S}^1} v^2 (\kappa_q - C(v))^2 dt + \int_{\mathbb{S}^1} \varepsilon v'^2 + \frac{1}{\varepsilon} \Phi(v) dt + \varepsilon \int_{\mathbb{S}^1} \kappa_q^2 dt, \quad (1.4)$$

where $\Phi : \mathbb{R} \rightarrow [0, \infty)$ is a continuous double-well potential, that is zero only in ± 1 and satisfies $\Phi(v) \rightarrow \infty$ as $v \rightarrow \pm\infty$. For notational simplicity we assume that Φ is symmetric with respect to the origin, and for technical reasons that it is C^2 in a neighbourhood of its minima. The function $C : \mathbb{R} \rightarrow \mathbb{R}$ is a continuous and bounded extension of $C(\pm 1)$.

The first integral in (1.4) resembles the curvature integral in (1.3); having the phase field in front of the curvature term enables the curves to approach kinks as $\varepsilon \rightarrow 0$. The third integral, however, penalises regions of very large curvature and accounts for a kink’s bending energy in the limit. Finally, interface costs are contributed by the second integral.

Below we show that the ε -energies (1.4) converge to (1.3) with

$$\sigma = 2 \int_{-1}^1 \sqrt{\Phi(v)} dv \quad \text{and} \quad \hat{\sigma} = 2\sqrt{\Phi(0)}. \quad (1.5)$$

In order to formulate and prove our theorem we fix these constants as in (1.5). We extend the energies \mathcal{E}_ε and \mathcal{E} to the space $H^1(\mathbb{S}^1; \mathbb{R}^2) \times L^1(\mathbb{S}^1)$ by setting $\mathcal{E}_\varepsilon(q, v) = \mathcal{E}(q, v) = \infty$ whenever (q, v) does not belong to $\mathcal{C}_\varepsilon \times \mathcal{P}_\varepsilon$ and $\mathcal{C} \times \mathcal{P}$, respectively.

Theorem 1.1. *The energies \mathcal{E}_ε are equi-coercive, that is any sequence $(q_\varepsilon, v_\varepsilon) \in \mathcal{C}_\varepsilon \times \mathcal{P}_\varepsilon$ with uniformly bounded energy admits a subsequence converging strongly in $H^1(\mathbb{S}^1; \mathbb{R}^2) \times L^1(\mathbb{S}^1)$ to some $(q, v) \in \mathcal{C} \times \mathcal{P}$.*

Furthermore, the \mathcal{E}_ε Γ -converge to \mathcal{E} as $\varepsilon \rightarrow 0$, that is

- for any sequence $(q_\varepsilon, v_\varepsilon)$ that converges to some (q, v) in $H^1(\mathbb{S}^1; \mathbb{R}^2) \times L^1(\mathbb{S}^1)$ as $\varepsilon \rightarrow 0$ we have

$$\liminf_{\varepsilon \rightarrow 0} \mathcal{E}_\varepsilon(q_\varepsilon, v_\varepsilon) \geq \mathcal{E}(q, v);$$

- for any (q, v) there is a sequence $(q_\varepsilon, v_\varepsilon)$ converging to (q, v) in $H^1(\mathbb{S}^1; \mathbb{R}^2) \times L^1(\mathbb{S}^1)$ such that

$$\limsup_{\varepsilon \rightarrow 0} \mathcal{E}_\varepsilon(q_\varepsilon, v_\varepsilon) \leq \mathcal{E}(q, v).$$

We postpone the proof of Theorem 1.1 to Section 2 in favour of some remarks and illustrations. Two examples of a local minimiser of \mathcal{E}_ε are given in Figure 1.1 for $\varepsilon = 0.05$ and $C(v)$ being a cubic interpolation of $C(-1) = 1$, $C(+1) = 2$, $C'(\pm 1) = 0$; the potential, and therewith the cost of kinks and interfaces, is $\Phi(v) = (1 - v^2)^2$ for the left pictures and $\Phi(v) = 0.75(1 - v^2)^2$ for the right. Both results are obtained by a gradient flow for \mathcal{E}_ε with respect to the H^{-1} norm for the phase field and the L^2 norm for the tangent angle; see [10, 8, 7] for details.

In both simulations the initial curve is a circle of radius 2 and the initial phase field has mean value zero with two interface regions. The interfaces are retained during the evolution, but new small areas of large curvature appear within the phase of spontaneous curvature 2. As already mentioned, these additional regions may persist as ε tends to zero, giving rise to ghost interfaces. Between (ghost) interfaces the numerically stationary curve consists of segments of circles whose curvatures are determined by the phase, but not equal to the preferred ones.

Our second note is the existence of minimisers for \mathcal{E} . From the properties of Γ -convergence and equi-coercivity, see for instance [4], we know that any sequence $(q_\varepsilon, v_\varepsilon) \in \mathcal{C}_\varepsilon \times \mathcal{P}_\varepsilon$ satisfying

$$\mathcal{E}_\varepsilon(q_\varepsilon, v_\varepsilon) = \inf_{\mathcal{C}_\varepsilon \times \mathcal{P}_\varepsilon} \mathcal{E}_\varepsilon + o(1),$$

admits a subsequence converging to a minimiser (q, v) of \mathcal{E} in $\mathcal{C} \times \mathcal{P}$. As the energy (1.4) is bounded from below, we can always find such almost minimising sequences. By the Direct Method of the Calculus of Variations there exists even a minimiser for each $\varepsilon > 0$, because \mathcal{E}_ε is coercive and weakly lower semi-continuous on $H^2(\mathbb{S}^1; \mathbb{R}^2) \times H^1(\mathbb{S}^1)$, and $\mathcal{C}_\varepsilon \times \mathcal{P}_\varepsilon$ is nonempty and weakly closed.

Finally, let us discuss three extensions of our theorem. First of all, the proof is easily adapted to non-symmetric potentials Φ . In this case one splits σ into two constants σ^\pm , defined as the integral of Φ over $(0, 1)$ and $(-1, 0)$, and distinguishes proper interfaces and ghost interfaces in different phases by their constant energy contribution $\sigma^+ + \sigma^-$, $2\sigma^+$ or $2\sigma^-$. One may also consider potentials like $\Phi(v) = (1 - v)^2$ and drop the volume constraint for v_ε . Then there is only one material phase, and the v_ε are mere auxiliary variables to allow curvature induced kinks.

Second, changing the power of ε in the last term of (1.4) to ε^k , $k > 1$, or even dropping the term completely yields the Γ -limit (1.3) with $\hat{\sigma} = 0$, that is, without bending contribution of kinks; the underlying topology changes to weak H^1 convergence of the curves.

Third, the arguments can be extended to handle non-closed curves with fixed end points and prescribed tangents in the approximate model. The additional issue in this situation is that kinks may appear at the boundary in the sense that the tangent vector of the limit curve differs from the prescribed one. As for ghost interfaces this yields a contribution to the limit energy; see [10] for the details.

2 Proof of Theorem 1.1

In this section we present the proof of Theorem 1.1. We first show equi-coercivity of the energies \mathcal{E}_ε , then establish the lower bound inequality and close with the upper bound. An important ingredient in what follows is the fact that given $q \in \mathcal{C}_\varepsilon$ and a directed line in the plane there is $u \in H^1(\mathbb{S}^1)$ such that $u(t)$ is the angle between $q'(t)$ and this line; u is uniquely determined up to adding multiples of 2π , and in addition we have $\kappa_q(t) = u'(t)$ for all $t \in \mathbb{S}^1$. On the other hand, the curve is uniquely determined by fixing one point together with its tangent there and an angle function. For $q \in \mathcal{C}$ we can still find an angle function $u \in H^1(\mathbb{S}^1 \setminus S_q)$, but as jumps can be arbitrarily large it is not unique anymore; of course we can assume that each jump is less than 2π . If we are only interested in finding a local angle function near a kink, its jump can be

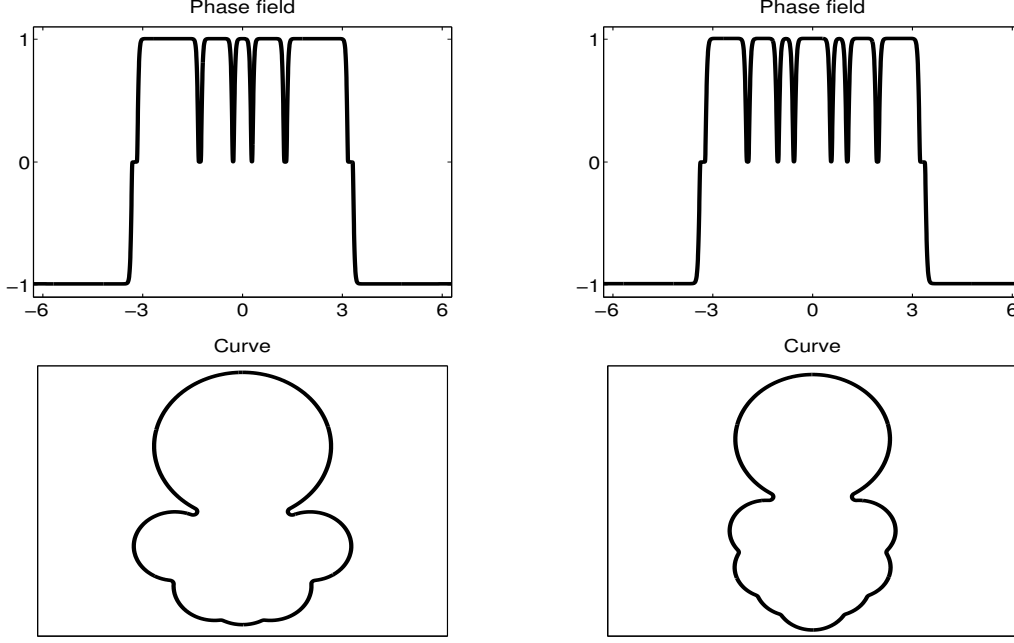


Figure 1.1: Two examples of numerically local minimisers of \mathcal{E}_ε . In the upper figures the phase fields are plotted over the sphere parametrised by the interval $[-2\pi, 2\pi]$; the lower figures show the curves in the xy -plane.

bounded by the enclosed angle of the limit tangents if the line is chosen appropriately. In such a local setting $||[q']||$ is simply given by $||[u]||$.

2.1 Equi-coercivity

Lemma 2.1. *Let $(q_\varepsilon, v_\varepsilon) \in \mathcal{C}_\varepsilon \times \mathcal{P}_\varepsilon$ be a sequence with uniformly bounded energy $\mathcal{E}_\varepsilon(q_\varepsilon, v_\varepsilon)$. Then there are $(q, v) \in \mathcal{C} \times \mathcal{P}$ and a subsequence, not relabelled, such that $q_\varepsilon \rightarrow q$ in $H^1(\mathbb{S}^1; \mathbb{R}^2)$ and $v_\varepsilon \rightarrow v$ in $L^1(\mathbb{S}^1)$.*

Furthermore, for this subsequence there are global angle functions $u_\varepsilon \in H^1(\mathbb{S}^1)$ that converge weakly in $BV(\mathbb{S}^1)$ to an angle function u of q .

Proof. The argument for the sequence of phase fields is based on well-known observations by Modica and Mortola, [14, 15] see in particular [4] for a proof in one dimension. The outcome is a finite set of points $\tilde{S} \subset \mathbb{S}^1$ and a function $v \in \mathcal{P}$ whose jump set S_v is contained in \tilde{S} such that a subsequence v_ε converges to v in measure and pointwise on $\mathbb{S}^1 \setminus \tilde{S}$. Moreover, in the one-dimensional setting (v_ε) is uniformly bounded in $L^\infty(\mathbb{S}^1)$, hence the subsequence converges in $L^p(\mathbb{S}^1)$ for any $p < \infty$; we also have $|v_\varepsilon| \geq 1/2$ for sufficiently small ε in any interval compactly contained in $\mathbb{S}^1 \setminus \tilde{S}$.

Taking into account only the just selected subsequence, we address the curves. As translations and rotations do not change the energy, we may assume that all curves pass at a fixed $s_0 \in \mathbb{S}^1$ through a common point with the same tangent vector τ_0 . From this and the fact that $|q'_\varepsilon| = 1$ we get $q_\varepsilon \rightarrow q$ in $H^1(\mathbb{S}^1; \mathbb{R}^2)$ for a subsequence. To show that $q \in H^2(\mathbb{S}^1 \setminus \tilde{S})$ let I be open and compactly contained in $\mathbb{S}^1 \setminus \tilde{S}$. As $v_\varepsilon^2 \geq 1/4$ in I for sufficiently small ε , the sequence $(\kappa_{q_\varepsilon}^2) = (|q''_\varepsilon|^2)$ is bounded in $L^1(I)$; thus a subsequence of (q''_ε) converges weakly in $L^2(I; \mathbb{R}^2)$ to some q''_I . But then q_ε converges weakly in $H^2(I; \mathbb{R}^2)$ and from uniqueness of the weak limit we infer that q''_I is the weak derivative of q' in I and that the whole sequence converges. This convergence combined with $|v_\varepsilon| \rightarrow 1$ and $\sup_\varepsilon \|v_\varepsilon\|_\infty < \infty$ yields the estimate

$$\int_I |q''_I|^2 dt \leq \liminf_{\varepsilon \rightarrow 0} \int_I v_\varepsilon^2 |q''_\varepsilon|^2 dt \leq \liminf_{\varepsilon \rightarrow 0} \int_{\mathbb{S}^1} v_\varepsilon^2 |q''_\varepsilon|^2 dt, \quad (2.1)$$

where the right hand side is bounded by the energy. Since (2.1) is true for any $I \Subset \mathbb{S}^1 \setminus \tilde{S}$, q'' , defined as q''_I on $I \Subset \mathbb{S}^1 \setminus \tilde{S}$, belongs to $L^2(\mathbb{S}^1; \mathbb{R}^2)$, and $q \in H^2(\mathbb{S}^1 \setminus \tilde{S}; \mathbb{R}^2)$ follows.

It remains to establish convergence of angle functions and to improve the convergence of the curves. Applying Hölder's inequality we get

$$\begin{aligned} \int_{\mathbb{S}^1} |\kappa_{q_\varepsilon}| dt &\leq \int_{\{|v_\varepsilon| < 1/2\}} |\kappa_{q_\varepsilon}| dt + \int_{\{|v_\varepsilon| \geq 1/2\}} |\kappa_{q_\varepsilon}| dt \\ &\leq \left(\int_{\mathbb{S}^1} \varepsilon \kappa_{q_\varepsilon}^2 dt \right)^{1/2} \left(\frac{1}{\varepsilon} |\{|v_\varepsilon| < 1/2\}| \right)^{1/2} + 2\sqrt{L} \left(\int_{\mathbb{S}^1} v_\varepsilon^2 \kappa_{q_\varepsilon}^2 dt \right)^{1/2}. \end{aligned}$$

Here the curvature integrals are bounded by $\mathcal{E}(q_\varepsilon, v_\varepsilon)$, and since Φ has a positive minimum on $[-1/2, 1/2]$, the quantity $|\{|v_\varepsilon| < 1/2\}|/\varepsilon$ is controlled by the potential energy. Hence, with \bar{u} satisfying $(\cos \bar{u}, \sin \bar{u}) = \tau_0$, the global angle functions

$$u_\varepsilon(s) = \bar{u} + \int_{s_0}^s \kappa_{q_\varepsilon}(t) dt$$

are uniformly bounded in $L^\infty(\mathbb{S}^1)$ and $W^{1,1}(\mathbb{S}^1 \setminus \{s_0\})$. Therefore there is a subsequence such that $u_\varepsilon \rightarrow u$ almost everywhere and weakly in $BV(\mathbb{S}^1)$, that is $u_\varepsilon \rightarrow u$ in $L^1(\mathbb{S}^1)$ and $\kappa_{q_\varepsilon} dt$ weakly to the measure Du . Consequently, $q'_\varepsilon = (\cos u_\varepsilon, \sin u_\varepsilon) \rightarrow (\cos u, \sin u) = q'$ in $L^2(\mathbb{S}^1; \mathbb{R}^2)$ and $q_\varepsilon \rightarrow q$ in $H^1(\mathbb{S}^1; \mathbb{R}^2)$. \square

2.2 Lower bound inequality

Next we prove the lower bound inequality

$$\liminf_{\varepsilon \rightarrow 0} \mathcal{E}_\varepsilon(q_\varepsilon, v_\varepsilon) \geq \mathcal{E}(q, v)$$

whenever $(q_\varepsilon, v_\varepsilon)$ converges to (q, v) in $H^1(\mathbb{S}^1; \mathbb{R}^2) \times L^1(\mathbb{S}^1)$. It suffices to examine the case when $(q_\varepsilon, v_\varepsilon) \in \mathcal{C}_\varepsilon \times \mathcal{P}_\varepsilon$ and to consider a subsequence such that the lower limit is attained. Then our compactness argument shows that $(q, v) \in \mathcal{C} \times \mathcal{P}$ and $S_q \cup S_v \subset \tilde{S}$, where $\tilde{S} \subset \mathbb{S}^1$ is a finite set of points. The same arguments as in (2.1) and the convergence $C(v_\varepsilon) \rightarrow C(v)$ in $L^2(\mathbb{S}^1)$ yield

$$\int_{\mathbb{S}^1 \setminus (S_q \cup S_v)} (\kappa_q - C(v))^2 dt \leq \liminf_{\varepsilon \rightarrow 0} \int_{\mathbb{S}^1} v_\varepsilon^2 (\kappa_{q_\varepsilon} - C(v_\varepsilon))^2 dt. \quad (2.2)$$

As points in $\tilde{S} \setminus (S_q \cup S_v)$ do not contribute to the limit energy, the task is to understand what happens near kinks and interfaces. To this end it is convenient to introduce the set-dependent energies

$$\mathcal{F}_\varepsilon(q_\varepsilon, v_\varepsilon, I) = \int_I \varepsilon v_\varepsilon'^2 + \frac{1}{\varepsilon} \Phi(v_\varepsilon) + \varepsilon \kappa_{q_\varepsilon}^2 dt$$

and

$$\mathcal{F}(q, v, I) = \sum_{s \in (S_q \cup S_v) \cap I} (\sigma + \hat{\sigma} |[q'](s)|)$$

for $I \subset \mathbb{S}^1$. In what follows we establish estimates for \mathcal{F}_ε and \mathcal{F} in the case of an interface without a kink, extend the argument to interfaces with a kink, and afterwards deal with ghost interfaces. The inequality for \mathcal{E}_ε and \mathcal{E} then follows by combining these estimates with (2.2).

2.2.1 Interfaces without kink: $s \in S_v \setminus S_q$

Let I be an open interval in \mathbb{S}^1 such that $\bar{I} \cap \tilde{S} = \{s\}$. As the curve q has no kink in I , it does not contribute to the limit energy $\mathcal{F}(q, v, I)$, so we estimate the curvature term of $\mathcal{F}_\varepsilon(q_\varepsilon, v_\varepsilon, I)$ simply by zero. The lower bound of the remaining part

$$\liminf_{\varepsilon \rightarrow 0} \int_I \varepsilon v_\varepsilon'^2 + \frac{1}{\varepsilon} \Phi(v_\varepsilon) dt \geq \sigma \quad (2.3)$$

is the well-known result for phase transitions by Modica and Mortola.[15, 14] In fact, there are points $a_\varepsilon, b_\varepsilon \in I$, $a_\varepsilon < s < b_\varepsilon$ or $b_\varepsilon < s < a_\varepsilon$ such that $v_\varepsilon(a_\varepsilon) \rightarrow -1$ and $v_\varepsilon(b_\varepsilon) \rightarrow 1$ for a subsequence $\varepsilon \rightarrow 0$; restricting the integral to $(a_\varepsilon, b_\varepsilon)$ or $(b_\varepsilon, a_\varepsilon)$, inequality (2.3) follows from Young's inequality and a substitution of variables.

2.2.2 Interfaces with kink: $s \in S_v \cap S_q$

Now let s be a point where the curve q has a kink and fix local angle functions u_ε in a small interval I around s such that \bar{I} contains no other point of \tilde{S} . By our equi-coercivity result we may assume that (u_ε) converges weakly in $BV(I)$ to an angle function u of q ; in particular, we have

$$\int_I u'_\varepsilon dt \rightarrow [u](s) + \int_I \kappa_q dt.$$

Note that $|[u](s)| \geq |[q'](s)|$ with strict inequality possible if the curves q_ε have loops near s that vanish in the limit.

We split the neighbourhood I of s into two parts: one where v_ε is close to zero and the other where its transition to ± 1 takes place; we expect q_ε to approximate the kink in the former part.

Lemma 2.2. *For I, u as above and any sufficiently small $\delta > 0$ let*

$$M_{\varepsilon, \delta} = \{t \in \mathbb{S}^1 : |v_\varepsilon(t)| \leq \delta\}$$

be the set where $|v_\varepsilon|$ is bounded by δ . Then

$$\liminf_{\varepsilon \rightarrow 0} \left| \int_{I \cap M_{\varepsilon, \delta}} u'_\varepsilon dt \right| \geq |[u](s)|.$$

Proof. Let $\gamma > 0$ be arbitrary but fixed, and let $U_\gamma := [s - \gamma, s + \gamma]$. As $I \setminus U_\gamma$ is compactly contained in $\mathbb{S}^1 \setminus \tilde{S}$ we have $|v_\varepsilon| \geq 2\delta$ in $I \setminus U_\gamma$ for all sufficiently small ε , and therefore $I \cap M_{\varepsilon, \delta} \subset U_\gamma$. Writing $w_\varepsilon = u'_\varepsilon - \kappa_q$, we have

$$\left| \int_{I \setminus M_{\varepsilon, \delta}} w_\varepsilon dt \right| \leq \left| \int_{I \setminus U_\gamma} w_\varepsilon dt \right| + \int_{(I \setminus M_{\varepsilon, \delta}) \cap U_\gamma} |w_\varepsilon| dt \quad (2.4)$$

for all sufficiently small ε . The first term in (2.4) converges to zero as $\varepsilon \rightarrow 0$ by weak convergence of $w_\varepsilon dt$ in $I \setminus U_\gamma$, and the second is less than a constant times $\sqrt{\gamma}$ due to Hölder's inequality and the energy bound. As $\gamma > 0$ is arbitrary we obtain

$$\limsup_{\varepsilon \rightarrow 0} \left| \int_{I \setminus M_{\varepsilon, \delta}} w_\varepsilon dt \right| = 0,$$

and taking the lower limit in the inequality

$$\left| \int_{I \cap M_{\varepsilon, \delta}} w_\varepsilon dt \right| \geq \left| \int_I w_\varepsilon dt \right| - \left| \int_{I \setminus M_{\varepsilon, \delta}} w_\varepsilon dt \right|$$

yields the claim as $\kappa_q \in L^2(I)$ and $|I \cap M_{\varepsilon, \delta}| \rightarrow 0$. \square

Next we prove the key estimate for the lower bound inequality at kinks.

Lemma 2.3. *Let $I \subset \mathbb{S}^1$ be an open interval such that \bar{I} contains exactly one point $s \in S_v \cap S_q$ and no other points of \tilde{S} . Then*

$$\liminf_{\varepsilon \rightarrow 0} \mathcal{F}_\varepsilon(q_\varepsilon, v_\varepsilon, I) \geq \hat{\sigma} |[q'](s)| + \sigma.$$

Proof. With the notation of Lemma 2.2 we have

$$\mathcal{F}_\varepsilon(q_\varepsilon, v_\varepsilon, I) \geq \int_{I \cap M_{\varepsilon, \delta}} \varepsilon u_\varepsilon'^2 + \frac{1}{\varepsilon} \Phi(v_\varepsilon) dt + \int_{I \setminus M_{\varepsilon, \delta}} \varepsilon v_\varepsilon'^2 + \frac{1}{\varepsilon} \Phi(v_\varepsilon) dt. \quad (2.5)$$

Estimating the first term with Hölder's and Young's inequality we get

$$\begin{aligned} \int_{I \cap M_{\varepsilon, \delta}} \varepsilon u_{\varepsilon}'^2 + \frac{1}{\varepsilon} \Phi(v_{\varepsilon}) dt &\geq \frac{\varepsilon}{|I \cap M_{\varepsilon, \delta}|} \left(\int_{I \cap M_{\varepsilon, \delta}} u_{\varepsilon}' dt \right)^2 + \frac{|I \cap M_{\varepsilon, \delta}|}{\varepsilon} \inf_{v \in [-\delta, \delta]} \Phi(v) \\ &\geq 2 \left| \int_{I \cap M_{\varepsilon, \delta}} u_{\varepsilon}' dt \right| \sqrt{\inf_{v \in [-\delta, \delta]} \Phi(v)}. \end{aligned}$$

With the second integral in (2.5) we deal as in the case before; the only difference is that we now find an interval $(a_{\varepsilon}, b_{\varepsilon}) \subset I \setminus M_{\varepsilon, \delta}$ such that $v_{\varepsilon}(a_{\varepsilon}) \rightarrow \delta$, $v_{\varepsilon}(b_{\varepsilon}) \rightarrow 1$ on one side of s , and the same with $-\delta$ and -1 on the other. Putting both estimates together and passing to the lower limit as $\varepsilon \rightarrow 0$ yields

$$\liminf_{\varepsilon \rightarrow 0} \mathcal{F}_{\varepsilon}(q_{\varepsilon}, v_{\varepsilon}, I) \geq 2|[u](s)| \sqrt{\inf_{v \in [-\delta, \delta]} \Phi(v)} + 2 \int_{\delta}^1 \sqrt{\Phi(v)} dv + 2 \int_{-1}^{-\delta} \sqrt{\Phi(v)} dv,$$

and taking the supremum over all $\delta > 0$ completes the proof. \square

2.2.3 Ghost interfaces: $s \in S_q \setminus S_v$

Finally, let $s \in S_q \setminus S_v$ and $I \subset \mathbb{S}^1$ such that $\bar{I} \cap \tilde{S} = \{s\}$ and the phase field v is constant in \bar{I} , say $v \equiv 1$. Then we argue as in Lemma 2.2 and 2.3 to find

$$\liminf_{\varepsilon \rightarrow 0} \mathcal{F}_{\varepsilon}(q_{\varepsilon}, v_{\varepsilon}, I) \geq \hat{\sigma} |[q'](s)| + 2 \cdot 2 \int_0^1 \sqrt{\Phi(v)} dv,$$

where the right-hand side is equal to $\hat{\sigma} |[q'](s)| + \sigma$ due to the symmetry of Φ . A similar argument is true when $v \equiv -1$ near s , and this concludes the proof of the lower bound estimate for $\mathcal{F}_{\varepsilon}$ and therewith $\mathcal{E}_{\varepsilon}$.

2.3 Upper bound inequality

The final subsection is devoted to the upper bound inequality. Given (q, v) with finite energy $\mathcal{E}(q, v)$, we find a recovery sequence $(q_{\varepsilon}, v_{\varepsilon})$ by changing (q, v) around (ghost) interfaces. For each $s \in S = S_q \cup S_v$ we choose two nested intervals of size of order ε : In the inner the kink is smoothed out by a linear interpolation of a local angle function, and in the outer the phase field transition to ± 1 is made. But we have to ensure not to violate any constraint and not to tear the curve apart when applying local changes to q and v .

2.3.1 The curve

Let $s \in S_q$ and $I \subset \mathbb{S}^1$ with $\bar{I} \cap S_q = \{s\}$. For simplicity of notation we identify points in I with coordinates that map s to the origin and formulate the following arguments for curves and phase fields given in an interval I around $s = 0$.

We fix a line passing through the kink so that the tangents $q'(t)$ as $t \rightarrow 0$ from above and below meet it with angle \bar{u} and $-\bar{u}$ for some $\bar{u} \in (0, \pi/2]$; then the kink carries the “bending energy” $2\bar{u}\hat{\sigma}$. The local angle function u corresponding to the line is uniformly continuous on either side of $t = 0$, hence by decreasing I we may assume that $|u| < \pi$ in I and that $u(t)$ is negative for $t < 0$ and positive for $t > 0$.

In the simple case that q is made up of two straight lines so that u is constant on either side of zero, the linear interpolation u_{ε} on an interval $I_{\varepsilon} = (-\delta_{\varepsilon}, \delta_{\varepsilon}) \subset I$ is given by

$$u_{\varepsilon}(t) = \begin{cases} -\bar{u} & : t < -\delta_{\varepsilon}, \\ \frac{\bar{u}}{\delta_{\varepsilon}} t & : |t| \leq \delta_{\varepsilon}, \\ \bar{u} & : t > \delta_{\varepsilon}, \end{cases}$$

where δ_{ε} is intended to go to zero as ε does. For the curve q_{ε} , defined by u_{ε} and one endpoint of $q_{\varepsilon}(I)$ equal to the corresponding endpoint of $q(I)$, we compute

$$\mathcal{F}_{\varepsilon}(q_{\varepsilon}, 0, I_{\varepsilon}) = 2 \frac{\varepsilon}{\delta_{\varepsilon}} \bar{u}^2 + 2 \frac{\delta_{\varepsilon}}{\varepsilon} \Phi(0) \geq 4\bar{u} \sqrt{\Phi(0)} = \hat{\sigma} |[q']|,$$

using Young's inequality, and equality holds if and only if

$$\delta_\varepsilon = \frac{\bar{u}}{\sqrt{\Phi(0)}}\varepsilon = \frac{|[q']|}{2\sqrt{\Phi(0)}}\varepsilon.$$

With this δ_ε we return to the general case: the linear interpolation of the angle on I_ε now is

$$u_\varepsilon(t) = \begin{cases} u(t) & : \delta_\varepsilon < |t|, \\ \frac{(u(\delta_\varepsilon) - u(-\delta_\varepsilon))}{2\delta_\varepsilon}t + \frac{(u(\delta_\varepsilon) + u(-\delta_\varepsilon))}{2} & : \delta_\varepsilon \geq |t|, \end{cases}$$

and similarly as above we get

$$\begin{aligned} \mathcal{F}_\varepsilon(q_\varepsilon, 0, I_\varepsilon) &= \frac{|u(\delta_\varepsilon) - u(-\delta_\varepsilon)|^2}{2\bar{u}}\sqrt{\Phi(0)} + 2\bar{u}\sqrt{\Phi(0)} \\ &\rightarrow 4\bar{u}\sqrt{\Phi(0)} = \hat{\sigma}[|q'|]. \end{aligned}$$

But as noted before, just replacing q by q_ε on I is not admissible since the second endpoint of $q(I)$ is not reached by $q_\varepsilon(I)$ and the whole curve would become discontinuous. Recalling the relation of tangent and angle function, the condition on the endpoints can be expressed as condition for u_ε by requiring

$$\begin{aligned} \int_I \cos u_\varepsilon(t) dt &= \int_I \cos u(t) dt =: C_0, \\ \int_I \sin u_\varepsilon(t) dt &= \int_I \sin u(t) dt =: S_0. \end{aligned} \tag{2.6}$$

We amend the linear interpolation u_ε by adding a perturbation that on the one hand is sufficiently small not to contribute to the energy in the limit $\varepsilon \rightarrow 0$, but on the other hand corrects the defect in the constraints (2.6). We will find two smooth functions f and g , which depend on u in I , and two parameters α_ε and β_ε such that $u_\varepsilon + \alpha_\varepsilon f + \beta_\varepsilon g$ is admissible for sufficiently small ε ; the argument is simply the Implicit Function Theorem applied to

$$P(\varepsilon, \alpha, \beta) := \begin{pmatrix} C_0 - \int_I \cos(u_\varepsilon + \alpha f + \beta g) dt \\ -S_0 + \int_I \sin(u_\varepsilon + \alpha f + \beta g) dt \end{pmatrix}.$$

Lemma 2.4. *Let q , u and u_ε be as above. There exist two functions $f, g \in C_0^\infty(I)$ such that there are $\varepsilon_0 > 0$ and functions $\varepsilon \mapsto \alpha_\varepsilon$, $\varepsilon \mapsto \beta_\varepsilon$, continuously differentiable in $[0, \varepsilon_0)$ that satisfy $P(\varepsilon, \alpha_\varepsilon, \beta_\varepsilon) = 0$ for all $\varepsilon \in [0, \varepsilon_0)$.*

Proof. Writing u as sum of a continuous function and a piecewise constant jump function and u_ε correspondingly, it is easily seen that P is a C^1 function for sufficiently small $\varepsilon \geq 0$. To apply the Implicit Function Theorem we have to show that $\partial_{(\alpha, \beta)} P(0, 0, 0)$ is non-singular. To this end we define two linear continuous functionals $T_s, T_c : C_0^\infty(I) \rightarrow \mathbb{R}$,

$$T_s \varphi = \int_I \varphi(t) \sin u(t) dt \quad \text{and} \quad T_c \varphi = \int_I \varphi(t) \cos u(t) dt,$$

and compute

$$\partial_{(\alpha, \beta)} P(0, 0, 0) = \begin{pmatrix} T_s f & T_s g \\ T_c f & T_c g \end{pmatrix}.$$

Assume for the moment that neither T_s nor T_c is constantly zero. Suppose for contradiction that $\ker T_s = \ker T_c$, which implies the existence of $\lambda \neq 0$ such that $T_s = \lambda T_c$; hence $\sin u = \lambda \cos u$ in I . This can only be true if u is piecewise constant, but then $\sin \bar{u} = \lambda \cos \bar{u}$ and $-\sin \bar{u} = \lambda \cos \bar{u}$ contradict each other due to $\lambda \neq 0$.

Thus $\ker T_s \neq \ker T_c$, say $\ker T_s \cap \ker T_c \subsetneq \ker T_c$, and there is $f \in \ker T_c$ such that $T_s f = 1$. After fixing any g with $T_c g = 1$, the partial derivative is

$$\partial_{(\alpha, \beta)} P(0, 0, 0) = \begin{pmatrix} 1 & * \\ 0 & 1 \end{pmatrix},$$

where $*$ is some real number. This matrix is non-singular, hence all prerequisites of the Implicit Function Theorem are satisfied and the claim is proved.

It remains to consider the situation when one of the operators is zero. This is certainly not T_s , since $T_s\varphi = 0$ for all $\varphi \in C_0^\infty(I)$ implies $\sin u = 0$ and, due to $|u| < \pi$, $u \equiv 0$ in I . There is, however, a valid situation such that $T_c = 0$, and that is if and only if $u(t) = \pi/2 \operatorname{sign} t$ is piecewise constant with a jump of height π . But then the second component of $P(\varepsilon, 0, \beta)$ is zero for all $\varepsilon \geq 0$, all $\beta \geq 0$ and any anti-symmetric function g . Fixing such g with $T_s g \neq 0$, we can thus apply the Implicit Function Theorem to $\tilde{P}(\varepsilon, \beta) = P_1(\varepsilon, 0, \beta)$ and get the desired result with $f = \alpha_\varepsilon = 0$. \square

So we have found an approximation $u_\varepsilon + \alpha_\varepsilon f + \beta_\varepsilon g$ on I that satisfies the constraints. Due to $\alpha_0 = \beta_0 = 0$, α_ε and β_ε converge to zero as $\varepsilon \rightarrow 0$; then $u_\varepsilon + \alpha_\varepsilon f + \beta_\varepsilon g \rightarrow u$ in $L^1(I)$ and \hat{q}_ε , defined by $u_\varepsilon + \alpha_\varepsilon f + \beta_\varepsilon g$ and the endpoints of $q(I)$, converges to q in $H^1(I; \mathbb{R}^2)$ and satisfies

$$\lim_{\varepsilon \rightarrow 0} \mathcal{F}(\hat{q}_\varepsilon, 0, I_\varepsilon) = \hat{\sigma}[[q']]. \quad (2.7)$$

As the number of kinks is finite, the construction can be made for each $s \in S_q$ on an interval I_ε^s .

2.3.2 Phase field recovery and energy estimates

Now we construct a recovery sequence for the phase field which is in line with q_ε from above. It is well-known, see for example [1], that the optimal profile for a transition of v_ε from -1 to $+1$ is obtained by minimising

$$G_\varepsilon(v) = \int_{\mathbb{R}} \varepsilon |v'|^2 + \frac{1}{\varepsilon} \Phi(v) dt$$

among functions v that satisfy $v(0) = 0$ and $v(\pm\infty) = \pm 1$. Indeed, setting $v_\varepsilon(t) = v(t/\varepsilon)$ we observe

$$G_\varepsilon(v_\varepsilon) = G_1(v) \geq 2 \int_{\mathbb{R}} \sqrt{\Phi(v)} v' dt = 2 \int_{-1}^1 \sqrt{\Phi(v)} dv = \sigma.$$

Equality holds if and only if $v' = \sqrt{\Phi(v)}$, which admits a local solution p with initial condition $p(0) = 0$ because $\sqrt{\Phi(\cdot)}$ is continuous. Obviously the constants $+1$ and -1 are a global super- and sub-solution of the problem, hence p can be extended to the whole real line. Since $\Phi(p) > 0$ for $p \in (-1, +1)$, $p(t)$ converges to ± 1 as $t \rightarrow \pm\infty$. Thus $p(t/\varepsilon)$ minimises G_ε . Due to the symmetry of Φ we can presume $-p(-t) = p(t)$ and need to know the profile only for $t \geq 0$.

We assume again, that by identification with appropriate coordinates the (ghost) interface is located at $s = 0$ and that the phase field is given on an interval I containing s . The building block for the recovery sequence is

$$p_\varepsilon(t) = \begin{cases} 0 & : 0 \leq t \leq \delta_\varepsilon, \\ p\left(\frac{t-\delta_\varepsilon}{\varepsilon}\right) & : \delta_\varepsilon < t \leq \delta_\varepsilon + \sqrt{\varepsilon}, \\ p(1/\sqrt{\varepsilon}) + \frac{1}{\varepsilon}(t - \delta_\varepsilon - \sqrt{\varepsilon}) & : \delta_\varepsilon + \sqrt{\varepsilon} < t \leq \delta_\varepsilon + \sqrt{\varepsilon} + \varepsilon(1 - p(1/\sqrt{\varepsilon})), \\ 1 & : \delta_\varepsilon + \sqrt{\varepsilon} + \varepsilon(1 - p(1/\sqrt{\varepsilon})) < t, \end{cases}$$

which connects $p_\varepsilon = 0$ and $p_\varepsilon = 1$ by a transition according to the optimal profile and a linear function, see Figure 2.1; the length of $\{p_\varepsilon = 0\}$ is chosen consistently with the recovery of the curve, that is $\delta_\varepsilon = |[q'](0)|/(2\sqrt{\Phi(0)}) \cdot \varepsilon$. In the next lemma we estimate the interface energy of the nonzero part of p_ε .

Lemma 2.5. *For any curve $q \in H^2(I \setminus \{0\}; \mathbb{R}^2)$ we have*

$$\limsup_{\varepsilon \rightarrow 0} \mathcal{F}_\varepsilon(q, p_\varepsilon, I \cap \{t > \delta_\varepsilon\}) \leq \frac{\sigma}{2}.$$

Proof. The curve satisfies $\kappa_q \in L^2(I)$, so the integral of $\varepsilon \kappa^2$ vanishes as $\varepsilon \rightarrow 0$. The other terms are for sufficiently small ε easily estimated by

$$\int_{I \cap \{t > \delta_\varepsilon\}} \varepsilon |p'_\varepsilon|^2 + \frac{1}{\varepsilon} \Phi(p_\varepsilon) dr \leq \int_0^{1/\sqrt{\varepsilon}} |p'(r)|^2 + \Phi(p(r)) dr + (1 - p(1/\sqrt{\varepsilon})) (1 + \sup_{[0,1]} \Phi).$$

Taking the upper limit $\varepsilon \rightarrow 0$ and recalling the symmetry of Φ yield the result. \square

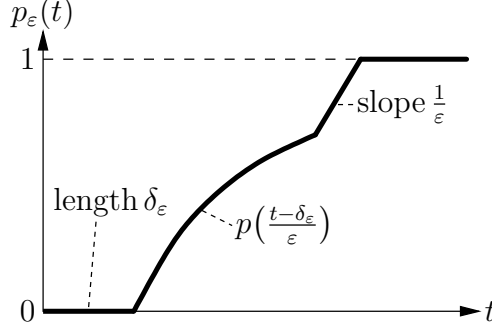


Figure 2.1: Construction of p_ε , consisting of space for the curve recovery, the optimal profile and the connection to 1.

It is now evident how to construct the recovery sequence for an interface: we simply take

$$v_\varepsilon(t) = \begin{cases} p_\varepsilon(t) & : 0 \leq t, \\ -p_\varepsilon(-t) & : 0 > t \end{cases}$$

or the negative of it. Then v_ε converges to v in $L^1(I)$; it follows from Lemma 2.5 that these approximations demonstrate the desired energy behaviour; in addition the volume constraint is not affected by substituting v_ε for v due to symmetry of p_ε .

In the case of a ghost interface we use the combination of $p_\varepsilon(t)$ and $p_\varepsilon(-t)$ or its negative. Again, convergence and energy behaviour are as required, but the volume constraint is violated. To get an admissible recovery sequence we add a small correction as we did with the angle function. Let $h : I \rightarrow \mathbb{R}$ be smooth, have compact support in $I \cap \mathbb{R}_{>0}$ and satisfy $\int_I h \, dt = 1$. Then the volume constraint is satisfied by $v_\varepsilon + \gamma_\varepsilon h$, if

$$\gamma_\varepsilon = \int_I v - v_\varepsilon \, dt.$$

Since

$$\int_{\delta_\varepsilon}^{\delta_\varepsilon + \sqrt{\varepsilon}} 1 - p_\varepsilon \, dt = \sqrt{\varepsilon} \int_0^1 1 - p(t/\sqrt{\varepsilon}) \, dt = o(\sqrt{\varepsilon}),$$

γ_ε is of order $o(\sqrt{\varepsilon})$, too. This is enough to still ensure convergence $v_\varepsilon + \gamma_\varepsilon h \rightarrow v$ in $L^1(I)$ and the energy inequality

$$\limsup_{\varepsilon \rightarrow \infty} \mathcal{F}_\varepsilon(q, p_\varepsilon + \gamma_\varepsilon h, I \cap \{t > \delta_\varepsilon\}) \leq \frac{\sigma}{2}, \quad (2.8)$$

thanks to

$$\frac{1}{\varepsilon} \Phi(\pm 1 + \gamma_\varepsilon h) = \frac{1}{\varepsilon} (\Phi(\pm 1) + \gamma_\varepsilon h \Phi'(\pm 1) + O(\gamma_\varepsilon^2)) = o(1).$$

Therefore v can be recovered around each interface, and the sequence for v on \mathbb{S}^1 is now built by substituting $v_\varepsilon + \gamma_\varepsilon h$ locally for v . Combining the constructions for phase field and curve we have the following result.

Corollary 2.6. *For $(q, v) \in \mathcal{C} \times \mathcal{P}$ and sufficiently small ε there is $(q_\varepsilon, v_\varepsilon) \in \mathcal{C}_\varepsilon \times \mathcal{P}_\varepsilon$ such that $q_\varepsilon \rightarrow q$ in $H^1(\mathbb{S}^1; \mathbb{R}^2)$, $v_\varepsilon \rightarrow v$ in $L^1(\mathbb{S}^1)$ and*

$$\limsup_{\varepsilon \rightarrow 0} \mathcal{E}_\varepsilon(q_\varepsilon, v_\varepsilon) \leq \mathcal{E}(q, v).$$

Proof. Denote by q_ε and v_ε the recovery sequences from this subsection. The convergence results have already been established; for the inequality note that for each $s \in S$ we have intervals $I_\varepsilon^s \subset I^s$ such that the kink is smoothed out in I_ε^s and the phase field transition is made in $I^s \setminus I_\varepsilon^s$; so combining the estimates (2.7) and (2.8) we get

$$\limsup_{\varepsilon \rightarrow 0} \mathcal{F}_\varepsilon(q_\varepsilon, v_\varepsilon, I^s) = \limsup_{\varepsilon \rightarrow 0} (\mathcal{F}_\varepsilon(q_\varepsilon, 0, I_\varepsilon^s) + \mathcal{F}_\varepsilon(q, v_\varepsilon, I^s \setminus I_\varepsilon^s)) \leq \mathcal{F}(q, v, I^s). \quad (2.9)$$

Outside $J := \bigcup_{s \in S} I^s$ phase field and curve remain unchanged, therefore

$$\limsup_{\varepsilon \rightarrow 0} \mathcal{F}_\varepsilon(q_\varepsilon, v_\varepsilon, \mathbb{S}^1 \setminus J) = \limsup_{\varepsilon \rightarrow 0} \mathcal{F}_\varepsilon(q, v, \mathbb{S}^1 \setminus J) = 0.$$

Together with (2.9) summed over all $s \in S$ this yields the upper bound inequality for $\mathcal{F}_\varepsilon(q_\varepsilon, v_\varepsilon, \mathbb{S}^1)$ and $\mathcal{F}(q, v, \mathbb{S}^1)$. Finally, because v_ε is zero where κ_{q_ε} differs from κ_q by more than the small correction for the endpoint constraints, we have

$$\begin{aligned} \int_{\mathbb{S}^1} v_\varepsilon^2 (\kappa_{q_\varepsilon} - C(v_\varepsilon))^2 dt &\leq \int_{\mathbb{S}^1 \setminus \bigcup I_\varepsilon^s} (\kappa_q - C(v_\varepsilon))^2 dt + o(1) \\ &\leq \int_{\mathbb{S}^1 \setminus S} (\kappa_q - C(v_\varepsilon))^2 dt + o(1), \end{aligned}$$

and taking the upper limit finishes the proof. \square

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